

chain nodes:

7 9 11

ring nodes:

1 2 3 4 5 6

ring/chain nodes:

10 12

chain bonds:

4-7 6-9 9-10 10-11 11-12

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:

1-2 1-6 2-3 3-4 4-5 4-7 5-6 6-9 9-10 10-11 11-12

isolated ring systems:

containing 1:

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS9:CLASS10:CLASS11:CLASS12:CLASS